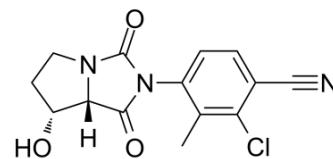


## BMS-564929

Cat. No.:	HY-12111		
CAS No.:	627530-84-1		
Molecular Formula:	C <sub>14</sub> H <sub>12</sub> ClN <sub>3</sub> O <sub>3</sub>		
Molecular Weight:	305.72		
Target:	Androgen Receptor		
Pathway:	Others		
Storage:	Powder	-20°C	3 years
		4°C	2 years
	In solvent	-80°C	6 months
		-20°C	1 month



### SOLVENT & SOLUBILITY

**In Vitro**  
 DMSO : 50 mg/mL (163.55 mM; Need ultrasonic)  
 H<sub>2</sub>O : < 0.1 mg/mL (insoluble)

Preparing Stock Solutions	Solvent Concentration	Mass		
		1 mg	5 mg	10 mg
	1 mM	3.2710 mL	16.3548 mL	32.7097 mL
	5 mM	0.6542 mL	3.2710 mL	6.5419 mL
	10 mM	0.3271 mL	1.6355 mL	3.2710 mL

Please refer to the solubility information to select the appropriate solvent.

**In Vivo**

- Add each solvent one by one: 10% DMSO >> 40% PEG300 >> 5% Tween-80 >> 45% saline  
 Solubility: ≥ 2.5 mg/mL (8.18 mM); Clear solution
- Add each solvent one by one: 10% DMSO >> 90% corn oil  
 Solubility: ≥ 2.5 mg/mL (8.18 mM); Clear solution

### BIOLOGICAL ACTIVITY

**Description** BMS-564929 is an androgen receptor (AR) agonist, binds to androgen receptor (AR) with a K<sub>i</sub> of 2.11±0.16 nM.

**IC<sub>50</sub> & Target** Ki: 2.11±0.16 nM (Androgen receptor)<sup>[1]</sup>

**In Vitro** BMS-564929 exhibits a potency (EC<sub>50</sub>, calculated as the concentration at which 50% of the maximum stimulatory effect of DHT is achieved) of 0.44±0.03 nM in the C2C12 myoblast cell line. In the PEC cell line, the EC<sub>50</sub> for BMS-564929 is 8.66±0.22 nM. BMS-564929 is more than 1000-fold selective for AR vs. estrogen receptors (ER) α and β, glucocorticoid receptor (GR), and mineralocorticoid receptor (MR), and approximately 400-fold selective vs.

progesterone receptor (PR). BMS-564929 shows no measurable activity in functional transactivation assays with ER  $\alpha/\beta$ , GR, MR, or PR at concentrations up to 30  $\mu\text{M}$ <sup>[1]</sup>.

#### In Vivo

In sexually mature, castrated male rats, a well-characterized animal model, BMS-564929 (p.o.) shows substantially more potent activity in the levator ani, exhibiting an  $\text{ED}_{50}$  of 0.0009 mg/kg in the levator ani and an  $\text{ED}_{50}$  of 0.14 mg/kg in the prostate; a net 160-fold selectivity for muscle vs. prostate. Approximately 100% muscle stimulation is achieved at 0.1 mg/kg, reaching greater than 125% stimulation at 0.3 and 1 mg/kg. Compared with T propionate (TP) in the same model, BMS-564929 is more than 200 times more potent in stimulation of muscle and 80 times more selective for muscle vs. prostate<sup>[1]</sup>.

## PROTOCOL

### Kinase Assay <sup>[1]</sup>

The human cancer epithelial breast cell lines MDA MB-453 and T47D, which endogenously express AR and progesterone receptor (PR), respectively, are used for radioligand competition binding assays. Binding assays are conducted by incubating BMS-564929 at various concentrations with either [<sup>3</sup>H]DHT or [<sup>3</sup>H]progesterone with the cells for 2 h at room temperature. For ER $\alpha$  and ER $\beta$ , fusion proteins expressed in Escherichia coli, consisting of maltose binding protein, a specific biotinylation sequence, an enterokinase cleavage site, and either the ER $\alpha$  or ER $\beta$  LBD is used. Binding reactions are conducted by incubating ER $\alpha$  and ER $\beta$  LBD with BMS-564929 and [<sup>3</sup>H]E2 for 2 h at room temperature. Specific binding activity to the mineralocorticoid receptor (MR) by BMS-564929 is evaluated by competition binding assay using kidney cytosolic preparations and [<sup>3</sup>H]aldosterone. The kidneys are obtained from adrenalectomized rats to remove the endogenous source of aldosterone and to increase the MR concentration in the cytosol of kidney cells. Binding reactions are incubated for 2 h on ice in the presence of excess mifepristone (RU486) to block nonspecific glucocorticoid receptor (GR) binding. A fluorescence polarization based assay is used for GR binding, as per manufacturer recommendations. Inhibitory constants ( $K_i$ , app) defining apparent binding affinity of test compounds to intracellular receptors are calculated from the observed inhibition of natural ligand binding at multiple concentrations of test compound. SHBG binding is performed using a standard charcoal assay. Reagents: 1 mg lyophilized SHBG powder (Tris), [<sup>3</sup>H]DHT, 3% charcoal, and 0.4% Dextran in PBS; binding buffer: 50 mM Tris, pH 7.6, 100 mM NaCl, 1 mM EDTA, 1 mM DTT, and mock lysate (3.5  $\mu\text{g}/100 \mu\text{L}$  buffer); stock solutions: stock SHBG protein: 1 mg/mL in water=20  $\mu\text{M}$ ; stock [<sup>3</sup>H]DHT ligand: 9  $\mu\text{M}$ ; DHT: 10 mM in DMSO; BMS 564929: 10 mM in DMSO. Compounds diluted in binding buffer are added to 40 nM [<sup>3</sup>H]DHT and 20 nM SHBG protein in 200  $\mu\text{L}$  volume and incubated for 1 h at room temperature. Total binding: 40 nM [<sup>3</sup>H]DHT and 20 nM SHBG protein in 200  $\mu\text{L}$  volume; nonspecific binding: 40 nM [<sup>3</sup>H]DHT and 20 nM SHBG protein and 1 mM cold DHT in 200  $\mu\text{L}$  volume. At the end of the incubation period, 200  $\mu\text{L}$  of the charcoal solution (3% containing 0.04% dextran) is added to 200  $\mu\text{L}$  of the reactions and shaken for 15 min before centrifugation. Supernatant (200  $\mu\text{L}$ ) is then transferred to the wells of a 24-well white Optiplate; 200  $\mu\text{L}$  of scintillant are added with mixing. Radioactivity counts are read in Topcount<sup>[1]</sup>. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

### Animal Administration <sup>[1]</sup>

Rats<sup>[1]</sup>  
Matched sets of castrated, sexually mature Harlan Sprague Dawley rats (42-56 d old, 200-250 g) are dosed once daily by oral gavage with BMS-564929 (0.00001-10 mg/kg) in solution/suspension of 80% PEG 400 and 20% Tween 20 for 14 d. Two control groups, one sham operated intact and one castrated, are dosed orally with the PEG/TW vehicle only, beginning on d 15 after surgery. Animals are dosed (vol/wt) at 1 mL/kg body weight. T propionate (TP) is dosed once daily sc in a 10% ethanol/90% peanut oil vehicle as a reference compound (0.03-10 mg/kg). After 14 d of treatment, the animals are killed by carbon dioxide asphyxiation, the levator ani and the ventral prostate are surgically removed and weighed, and serum is collected for LH measurements. MCE has not independently confirmed the accuracy of these methods. They are for reference only.

## CUSTOMER VALIDATION

- **Food Chem.** 2019 Sep.
- **J Chromatogr A.** 2019 Aug 30;1600:183-196.
- **Food Addit Contam Part A Chem Anal Control Expo Risk Assess.** 2020 May 13;1-11.
- **MethodsX.** 2020 May 23.

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## REFERENCES

[1]. Ostrowski J, et al. Pharmacological and x-ray structural characterization of a novel selective androgen receptor modulator: potent hyperanabolic stimulation of skeletal muscle with hypostimulation of prostate in rats. *Endocrinology*. 2007 Jan;148(1):4-12.

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**Caution: Product has not been fully validated for medical applications. For research use only.**

Tel: 609-228-6898

Fax: 609-228-5909

E-mail: [tech@MedChemExpress.com](mailto:tech@MedChemExpress.com)

Address: 1 Deer Park Dr, Suite Q, Monmouth Junction, NJ 08852, USA